CAMP: A Scalable, Portable, Gas–Aerosol Chemistry Treatment for Atmospheric Models

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1. What is CAMP?

- **CAMP is Chemistry Across Multiple Phases.**
- **CAMP** solves multi-phase chemical systems in atmospheric models.
- **CAMP** is being developed as part of the PartMC science library (https://github.com/compdyn/partmc).
- The initial deployment of **CAMP** is in the **MONARCH**[6] chemical weather prediction system and the **PartMC**[4] particle-resolved aerosol model (papers in preparation).

2. Motivation

- Incorporating increasingly complex chemistry into existing atmospheric models is challenging because of the large number of chemistry and 'chemistry-adjacent' sub-modules typically employed, their intricate (often hard-coded) interdependence, and the effects of operator splitting (Fig. 1).
- We are developing the CAMP model to ease this process by being:
  - **portable**: useable as a stand-alone library able to interact with any model's internal configuration, including how it represents aerosol systems.
  - **flexible**: fully run-time configurable chemical mechanisms requiring no changes to the source code or re-compilation of the model.
  - **self-contained**: solves the complete chemical system, including gas- and condensed-phase reactions and phase transfer as a single kinetic system.

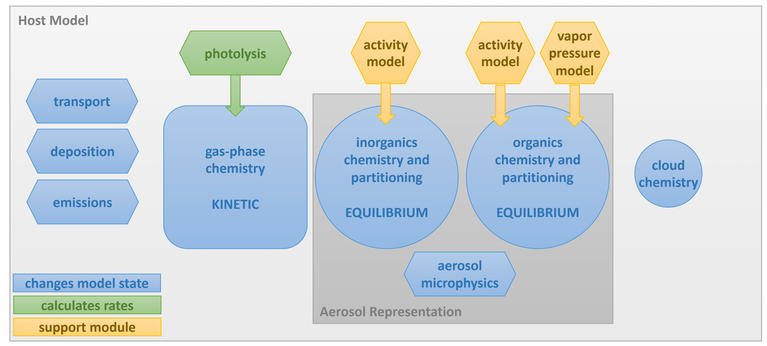


*Fig. 1: Configuration of chemistry and related modules in a typical atmospheric model. Multiple components directly update the model state (**blue**) and many are tightly tied to the aerosol representation used by the host model (**grey**; e.g., bins, modes, single-moment, double-moment, particle-resolved).*

3. Input data

- CAMP uses **JSON** input files (www.json.org), a widely used format for semi-structured data.
- CAMP accepts **three types of model elements** to build a mechanism, all of which are configured at run-time using JSON input files (Fig. 2):
  - **reactions**: gas-phase, condensed-phase, and partitioning (e.g., Henry's Law-based, SIMPOL[1] vapor pressure based).
  - **aerosol representations**: describing, for example, the single-particle or bin/mode structure of a model.
  - **sub-models**: used to calculate, for example, activity coefficients (PD-FiTE[2], UNIFAC[3]).

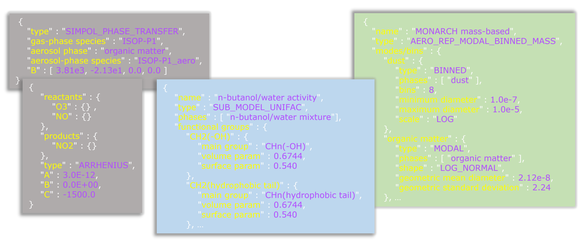
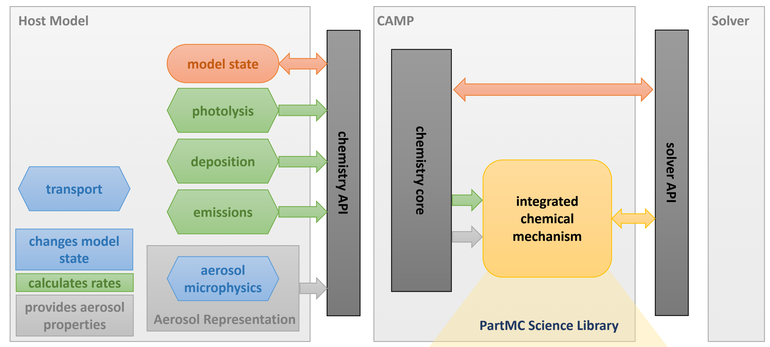


*Fig. 2: CAMP input data in JSON format for reactions (**grey**), aerosol representations (**green**) and sub-models (**blue**).*

4. Model Design

- CAMP interacts with a host atmospheric model through a **common API**.
- CAMP employs an **external solver**, currently SUNDIALS-CVODE[5], an implicit solver useful for mathematically stiff systems, like those treated by CAMP.
- Sub-modules that formerly directly updated the model state (e.g., emissions and deposition; Fig.1) now provide rates to CAMP (Fig.3) through the API. This, coupled with the integration of gas- and aerosol-phase reactions and partitioning, permits the **combined solving of the full chemical system**.
- An **object-oriented design** allows extension of three abstract model-element classes (**reactions**, **aerosol representations**, and **sub-models**), which provide functions needed during solving and are initialized using a set of JSON input data processed at run-time during model initialization.

The CAMP ground: how CAMP fits into your model



how CAMP describes chemical systems

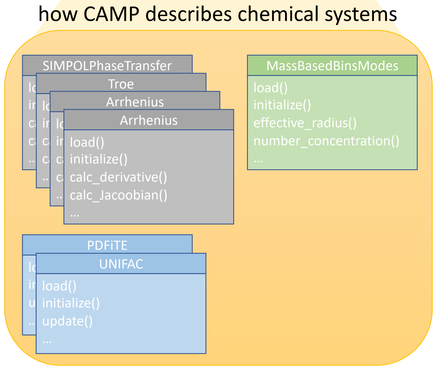


Fig. 3: Modified model configuration showing CAMP integration and internal chemical mechanism description.

5. CAMP GPU

- The flexible design of CAMP allows **multiple grid cells to be solved** as a combined chemical system.
- **Combined grid cell solving** has resulted in a speedup of up to a **factor of 12** under certain conditions.
- CAMP is also being ported to **mixed CPU/GPU systems** for optimized solving.
- For example, individual reaction equations for a mechanism of **100 reactions** and **1000 grid cells** can be spread across **10^5 GPU** threads for simultaneous calculation.

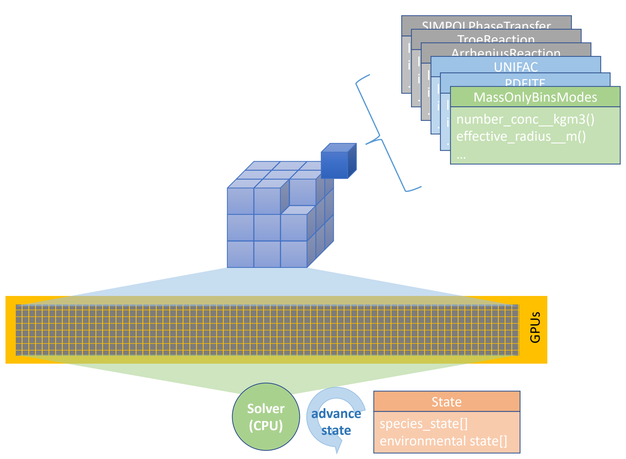


Fig. 4: Cartoon depicting the porting of individual calculations for a chemical mechanism (upper right) applied to a 3-D multiple grid cell system (blue cubes) to GPUs (grey squares) for solving.

6. Unit Tests

- Every CAMP model element has an associated unit test that solves a simple mechanism that can be **solved analytically** or compared to **published data** (for more complex model elements).

Some CAMP Model Elements	Test Type
Arrhenius	analytical
Troe (Fall-off)	analytical
HL Partitioning	analytical
SIMPOL.1 VP Partitioning	analytical/ published scenario[1]
Condensed-Phase Reversible	analytical
UNIFAC	analytical/ published scenario[3]
PD-FiTE	analytical/ published scenario[2]

References

1 Pankow, J. F., & Asher, W. E. (2008). *Atmos. Chem. Phys.*, 8(10), 2773–2796.
2 Topping, D., Lowe, D., & McFiggans, G. (2009). *J. Geophys. Res.*, *114*(D04304), 1–13. https://doi.org/10.1029/2008JD010099.
3 Marcolli, C., & Peter, T. (2005). *Atmos. Chem. Phys.*, *5*, 1545–1555.
5 West M., Riemer N., Curtis J., Michelotti M., and Tian J. (2018) PartMC, v2.5.0, DOI 10.5281/zenodo.1490925
6 Hindmarsh, A. et al. (2005) *ACM TOMS*, 31(3), 363–396.
7 Badia, et. al. (2017) *Geosci. Model Dev.*, 10(2), 609–638.

Code availability

CAMP will be included in an upcoming release of the PartMC science library, available at: https://github.com/compdyn/partmc

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